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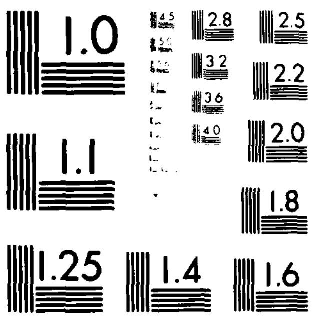

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FINAL SCIENTIFIC REPORT

Air Force Office of Scientific Research Grant AFOSR-80-0235

Period: 1 July 1980-30 June 1981

Title of Research: Applications of Invariant Imbedding

Principal Investigator: Paul Nelson

DTIC FILE COPY

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFOSR-TR- 82 -0028	2. GOVT ACCESSION NO. AD-A110	3. RECIPIENT'S CATALOG NUMBER 543
4. TITLE (and Subtitle) APPLICATIONS OF INVARIANT IMBEDDING		5. TYPE OF REPORT & PERIOD COVERED FINAL, 1 JUL 80 - 30 JUN 81
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Paul Nelson		8. CONTRACT OR GRANT NUMBER(s) AFOSR-80-0235
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Mathematics Texas Tech University Box 4139, Lubbock TX 79409		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F; 2304/A3
11. CONTROLLING OFFICE NAME AND ADDRESS Mathematical & Information Sciences Directorate Air Force Office of Scientific Research Bolling AFB DC 20332		12. REPORT DATE DEC 81
		13. NUMBER OF PAGES 16
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Invariant imbedding is a method for the computational solution of two-point boundary-value problems. One common source of such problems is in the application of the method of lines, or an expansion procedure, to a system of partial differential equations. Such partial differential equations might describe, for example, the dynamic mechanics of structures such as an aircraft fuselage or a missile silo.
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The research conducted under this grant has been directed toward two objectives. The first objective was to improve the effectiveness and efficiency of invariant imbedding by providing means for automatically controlling the associated computational effort. The second objective was to extend the range of applicability of invariant imbedding to include singular two-point boundary-value problems. Such singular problems arise, for example, by applying the method of lines to partial differential equations in spherical or cylindrical coordinate systems.

In regard to the first of these objectives, a number of different methods, which are generically termed 'relative-error monitors', have been developed and are in the process of being subjected to computational experimentation. As regards the second objective, it has been shown how to apply the method of invariant imbedding to 'homogeneous' linear two-point boundary-value problems. The further extension to inhomogeneous problems is presently being pursued.

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ABSTRACT

Invariant imbedding is a method for the computational solution of two-point boundary-value problems. One common source of such problems is in the application of the method of lines, or an expansion procedure, to a system of partial differential equations. Such partial differential equations might describe, for example, the dynamic mechanics of structures such as an aircraft fuselage or a missile silo.

The research conducted under this grant has been directed toward two objectives. The first objective was to improve the effectiveness and efficiency of invariant imbedding by providing means for automatically controlling the associated computational error within a minimal, or at least reasonable, degree of computational effort. The second objective was to extend the range of applicability of invariant imbedding to include singular two-point boundary-value problems. Such singular problems arise, for example, by applying the method of lines to partial differential equations in spherical or cylindrical coordinate systems.

In regard to the first of these objectives, a number of different methods, which are generically termed *relative-error monitors*, have been developed and are in the process of being subjected to computational experimentation. As regards the second objective, it has been shown how to apply the method of invariant imbedding to *homogeneous* linear two-point boundary-value problems. The further extension to inhomogeneous problems is presently being pursued.

RESEARCH OBJECTIVES AND STATUS

The work described here was concerned with automatic error control for invariant imbedding and with the extension of invariant imbedding to permit solution of singular linear two-point boundary-value problems. Progress on these two topics is discussed separaely in the following two subsections.

Automatic Error Control

The solutions of the initial-value problem which typically is integrated numerically in applications of invariant imbedding are usually not themselves the object of ultimate interest. Rather, these are intermediate quantities which are used via linear algebraic computations to approximate the solution of an underlying linear two-point boundary-value problem. Because of this situation, it is not readily apparent how to use modern adaptive initial-value integration techniques efficiently and effectively within invariant imbedding.

Nelson and Wiggins [1] studied one method of error control for initial-value integrations which was specifically designed for the version of invariant imbedding due to M.R. Scott [2-5]. In the work reported here we view this earlier approach as one of a class of methods, each of which is defined by quantities which we term *relative-error monitors* and associated *sensitivity functions*. Each such set of quantities provides a mechanism for approximately controlling that part of the error in the approximate solution of the underlying two-point boundary-value problem which stems from the initial-value integration. We now describe this approach to error control in some detail.

Consider a linear two-point boundary-value problem (TPBVP) of the form

$$u'(z) = A(z)u(z) + B(z)v(z) + s_+(z), \tag{1a}$$

$$v'(z) = C(z)u(z) + D(z)v(z) + s_-(z), \tag{1b}$$

$$u(0) = a, \; v(x) = b. \tag{1c}$$

Here u and v are respectively m and n- dimensional vectors of dependent variables, A,B,C and D are given piecewise continuous mattices of the appropriate dimensions, a and b are given vectors, and $x > 0$. If $0 \leq x < x_c$, where x_c is the smallest value of x such that (1) fails to have a unique solution (i.e. x_c is the smallest eigenlength of (1)), then the solution of (1) is given by

$$v(z) = T^{-1}(z)\{T(x)b + q_\ell(x) - q_\ell(z)\}, \tag{2a}$$

$$u(z) = R(z)v(z) + q_r(z), \tag{2b}$$

where R, T, q_r and q_ℓ are determined by the initial-value problem (IVP)

$$R' = B + AR - RD - RCR, \; R(0) = 0, \tag{3a}$$

$$T' = -T(CR+D), \; T(0) = I \text{ (= identity matrix)}, \tag{3b}$$

$$q_r' = (A-RC)q_r - Rs_- + s_+, \; q_r(0) = a, \tag{3c}$$

$$q_\ell' = -T(Cq_r + s_-), \; q_\ell(0) = 0. \tag{3d}$$

In applying (2) to the computational solution of the TPBVP (1), one normally integrates the IVP (3) from z=0 to z=x, with the values of R, T, q_r and q_ℓ at *reporting points* (= values of z at which it is ultimately desired to compute u and v) being stored during this integration. Once $T(x)$ and $q_\ell(x)$ have been computed, the approximations to u and v at the reporting points are then determined from (2) by appropriate numerical linear algebra. References 6-8 contain proofs of the assertions of the preceding paragraph or discussions of further computational considerations.

In contrast to the situation for IVP's, there is no generally accepted type of error criterion for TPBVP's. It would seem desirable to adopt a criterion of the form that at each reporting point at least one of the absolute or relative error should meet a specified tolerance. The difficulty with this basic idea lies in determining a reasonable measure of the magnitude of the solution in defining the relative error. It seems infeasible, or at least likely often to be inordinately expensive, to take this magnitude as some norm of the solution at the particular reporting point in question. As mentioned above, our approach is to introduce a class of relative-error monitors for the TPBVP (1), with each such monitor serving to provide a measure of the magnitude of the solution.

More specifically, a relative-error monitor for (1) is simply a real-valued function $M=M(z)$ such that

$$||v(z)|| \mathrel{\tilde{\leq}} M(z). \tag{4}$$

Given such a monitor, we take as our objective to control the errors δu and δv, in u and v respectively, so that

$$||\delta v(z)|| \mathrel{\tilde{\leq}} \varepsilon[1+M(z)] \tag{5a}$$

and

$$||\delta u(z)|| \mathrel{\tilde{\leq}} \varepsilon[(1+M(z))(1+||R(z)||)+||q_r(z)||] \tag{5b}$$

at each reporting point, where ε (= error tolerance) is specified prior to the computation. (We shall use δy to denote the error in a computational approximation to a quantity y. We ordinarily have the ∞-norm in mind, although in the spirit of our work it is immaterial which of the common vector norms is used, provided the dependent variables are properly scaled.

In consonance with our basic objective, we wish (5) to be implied by some type of control on the local truncation error associated with the numerical integration of the IVP (3). Toward that end, given a relative-error monitor for the TPBVP (1) we define associated *sensitivity functions* to be a quadruple of real-valued functions W_R, W_T, W_r and W_ℓ such that the inequalities

$$||\delta R(z)|| \leq \varepsilon W_R(z), \quad ||\delta T(z)|| \leq \varepsilon W_T(z), \tag{6a,b}$$

$$||\delta q_r(z)|| \leq \varepsilon W_r(z), \quad ||Sq_\ell(z)|| \leq \varepsilon W_\ell(z) \tag{6c,d}$$

imply (5). Given such sensitivity functions, the procedure is to integrate the IVP (3) so that (6) holds with the errors interpreted as the local truncation errors; if the IVP is computationally stable (and this should be checked by multiple numerical integrations), then (6) holds with the errors taken as the global errors, and therefore (5) is satisfied.

All of the following are, in the sense of the above definition, relative-error monitors for (1).

$$M_0(z) = ||T^{-1}(z)||\cdot\, ||T(x)||\cdot||b|| + ||q_\ell(x)|| + ||q_\ell(z)|| \;, \tag{7a}$$

$$M_1(z) = ||T^{-1}(z)T(x)||\cdot||b|| + ||T^{-1}(z)||\cdot||q_\ell(x)-q_\ell(z)||, \tag{7b}$$

$$M_2(z) = ||T^{-1}(z)||\cdot||T(x)b + q_\ell(x) - q_\ell(z)||, \tag{7c}$$

and

$$M_3(z) = ||v(z)||. \qquad (7d)$$

These are listed in order of increasing stringency of the associated requirement on the error in v. Sensitivity functions have been developed for all of these monitors. Computational experiments currently are being performed on a suite of test problems. The results will be reported in [9].

Singular Problems

The method of invariant imbedding has been widely applied to nonsingular TPBVP's, such as (1) of the preceding subsection, but little effort seems to have been devoted to its application to singular differential systems. Scott [1,Sec.V.8] considered sufficient conditions for existence of two different versions of invariant imbedding (the "r" and "s" equations) for linear second-order equations having a regular singular point. The work of Scott constitutes a significant extension of earlier results of Banks and Kurowski [10]. More recently, Elder [11] showed how to apply the subscheme of invariant imbedding known as integration-to-blowup [12,13] to compute the smallest eigenlength of a linear first-order system having a singularity of the first kind. The purpose of this work was to show how the approach of Elder can be extended to apply to the solution of certain singular two-point boundary-value problems by means of Scott's version [1-4] of invariant imbedding. The extension to *homogeneous* differential systems of the first kind has been completed, as reported in [14, 15]. Th further extension to inhomogeneous problems is in progress, and will be described in [16,17]. The application to homogeneous problems will now be described in some detail.

Consider a linear homogeneous first-order differential system with a singularity of the first kind at $z=0$,

$$u'(z) = \left(\frac{A_0}{z} + A(z)\right) u(z) + \left(\frac{B_0}{z} + B(z)\right) v(z), \tag{8a}$$

$$v'(z) = \left(\frac{C_0}{z} + C(z)\right) u(z) + \left(\frac{D_0}{z} + D(z)\right) v(z). \tag{8b}$$

Here u,v and A-D are as in the previous subsection, while A_0, B_0, C_0 and D_0 are constant matrices of the appropriate dimensions.

We wish to obtain solutions of (8) subject to boundary conditions of the form

$$u(0+) \text{ and } v(0+) \text{ exist (finite)} \tag{9a}$$

and

$$v(x) = \beta, \; x > 0. \tag{9b}$$

Let

$$Y(z) = \begin{pmatrix} Y_1(z) \\ Y_2(z) \end{pmatrix}, \tag{10}$$

be an $(m + n) \times q$ matrix the columns of which are a maximal linearly independent system of solutions of (1) subject to (2a), where Y_1 and Y_2 have respectively m and n rows. We define the $(m + n) \times (m + n)$ matrix E_0 by

$$E_0 = \begin{pmatrix} A_0 & B_0 \\ C_0 & D_0 \end{pmatrix}. \tag{11}$$

The salient results of [11] can then be summarized as follows:

Theorem A (Elder [11]): The number (q) of columns in the matrix Y(z) is equal to the dimension of the space H^+ *spanned by the eigenvectors and generalized eigenvectors of* E_0 *associated with eigenvalues* λ *satisfying* $Re(\lambda) > 0$ *along with the* <u>(proper)</u> *eigenvectors of* E_0 *associated with eigenvalue* $\lambda = 0$. *The two-point boundary-value problem (8), (9) has a unique solution if, and only if,* $q = n$ *and* $Y_2(x)$ *is an invertible matrix. If* $q = n$, *then* $Y_2(x)$ *is invertible (and hence (8), (9) has a unique solution) for all sufficiently small positive x if* H_n^+ *is invertible, where*

$$H = \begin{pmatrix} H_m^+ \\ H_n^+ \end{pmatrix} \tag{12}$$

is any $(m + n) \times n$ *matrix the columns of which constitute a basis for* H^+. *If there exists* $X > 0$ *such that (1), (2) has a unique solution for every x satisfying* $0 < x < X$, *then the matrix*

$$R(z) \equiv Y_1(z) Y_2(z)^{-1} \tag{13}$$

satisfies the Riccati differential equation

$$\left.\begin{aligned} R'(z) &= \left(\frac{B_0}{z} + B_1(z)\right) + \left(\frac{A_0}{z} + A_1(z)\right) R(z) \\ &-R(z)\left(\frac{D_0}{z} + D_1(z)\right) - R(z)\left(\frac{C_0}{z} + C_1(z)\right) R(z) \end{aligned}\right\} \tag{14}$$

for $z \varepsilon (0,X)$. *Furthermore, if* H_n^+ *is invertible, then*

$$R(0+) = H_m^+(H_n^+)^{-1}. \tag{15}$$

Henceforth we assume existence of some X as described in the statement of this theorem. The matrices H_m^+ and H_n^+ of (8) are, of course, of respective dimensions $m \times n$ and $n \times n$. We wish to emphasize that invertibility of H_n^+ implies our assumption (regarding X).

If Y_1 and Y_2 are as above, and u, v are any solution of the differential system (8) satisfying the regularity condition (9a), then is is readily shown that there exists a constant vector c such that

$$u(z) = Y_1(z)c, \; v(z) = Y_2(z)c. \tag{16a,b}$$

If additionally v satisfies the boundary-condition (9b), then (16b) along with invertibility of $Y_2(x)$ gives

$$c = Y_2(x)^{-1}\beta. \tag{17}$$

Thus if we define

$$T(z) = Y_2(z)^{-1} \tag{18}$$

then (16) can be combined to give

$$v(z) = T(z)^{-1}T(x)\beta, \; u(z) = R(z)v(z). \tag{19a.b}$$

Furthermore T is readily shown to satisfy the differential system

$$T'(z) = -T(z)\left(\frac{D_0}{z} + D_1(z)\right) + \left(\frac{C_0}{z} + C_1(z)\right) R(z) \quad . \tag{20}$$

Equations (19) are precisely analogous to the basic formulas used in determining the solution of a nonsingular (homogeneous) two-point boundary-value problem by means of Scott's version of invariant imbedding [1-4]. Furthermore (14) and (15) comprise an initial-value problem for R. Thus in order to reduce solution of (8), (9) to solution of initial-value problems and numerical linear algebra on matrices and vectors of order max(m,n) - which is the objective of any version of invariant imbedding - it remains only to determine the value of T(0), so that T can be obtained by numerical solution of the resulting initial-value problem (along with that for R).

At this juncture the simple analogy with the nonsingular situation breaks down, because it readily can happen that $Y_2(0)$ is noninvertible, so that T(0+) fails to exist. In fact, it also follows from results in Ref. 11 that $Y_2(0)$ is invertible if, and only if, the vector space H^+ of Theorem A consists entirely of eigenvectors of E_0 associated with the eigenvalue $\lambda = 0$. In this (likely rare) event one can simply take T(0) as any invertible $n \times n$ matrix (the identity matrix is certainly the simplest choice), because any such matrix is $Y_2(0)$ for some choice of Y(z). The values of R and T can then be obtained by numerical integration of the initial-value problem consisting of (14), (15) and (20), subject to the initial value selected for T.

In the case that $Y_2(0)$ is singular, the only general procedure we have found is as follows. It is readily shown that Y_2 satisfies the differential equation

$$Y_2'(z) = \left(\frac{C_0}{z} + C_1(z)\right) R(z) + \left(\frac{D_0}{z} + D_1(z)\right) Y_2(z). \tag{21}$$

For $0 \leq z \leq z_0$ one can then determine $R(z)$ and $Y_2(z)$ by numerical integration of the initial-value problem consisting of (14), (15), (21) and the initial condition

$$Y_2(0) = P_2 \ , \tag{22}$$

where

$$P = \begin{pmatrix} P_1 \\ P_2 \end{pmatrix}$$

is any $(m + n) \times n$ matrix the nonzero columns of which constitute a basis for the null space of E_0. With $Y_2(z_0)$ thus determined, $T(z_0) = Y_2(z_0)^{-1}$ can be obtained numerically. The required values of $R(z)$ and $T(z)$ for $z \geq z_0$ can then be obtained by numerical integration of (14) and (21) subject to the known values of $R(z_0)$ and $T(z_0)$. Alternately one could simply compute $Y_2(z)$ and $R(z)$ for all desired values of z, and then compute u and v by

$$v(z) = Y_2(z)Y_2(x)^{-1}\beta \tag{23}$$

and (19b).

There remains one further computational detail. Typical initial-value codes require the user to supply a subroutine which computes the derivative. However, the right-hand side of (14) is indeterminate at $z = 0$ for $R(0)$ given by (15) and (12), and likewise the right-hand of (20) (respectively (21)) in the case that $T(0)$ (respectively, $Y_2(0)$) exists. For the problems we have encountered it has been possible to determine $R'(0)$ and $Y_2'(0)$ (or $T'(0)$, when $T(0)$ exists) by applying L'Hospital's rule to (14) and (21) (or(20)), although we have no general proof of the effectiveness of this approach.

Several numerical examples illustrating the approach outlined above are presented in references 15 and 16. In addition the important special case of a single second-order equation is further studied in considerable detail, and several results specific to such problems are obtained.

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15. ____________________, Invariant Imbedding Applied to Homogeneous Two-Point Boundary-Value Problems with a Singularity of the First Kind, Appl. Math. Comput., to appear.

16. S.R. White, Invariant Imbedding Applied to Inhomogeneous Singular Two-Point Boundary-Value Problems, M.S. Report, Department of Mathematics, Texas Tech University, in preparation.

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CUMULATIVE LIST OF WRITTEN PUBLICATIONS

July 1, 1980 to date

Published Articles

P. Nelson and A.K. Ray, An Automatic Error-Control Technique for Computation of Eigenlengths, J. Comp. Phys. 37, 388-398 (1980).

P. Nelson and K.E. Wiggins, Automatic Control of Errors for Invariant Imbedding, Ordinary and Partial Differential Equations, W.N. Everitt and B.D. Sleeman Eds., Proceedings of the Sixth Dundee Conference on Differential Equations, Lecture Notes in Mathematics, Vol. 846, Springer-Verlag, Berlin, 1981, pp.253-263.

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I.T. Elder, Computation of Eigenlengths of Singular Two-Point Boundary-Value Problems by Invariant Imbedding, J. Math. Anal. Appl., to appear.

P. Nelson, I.T. Elder and S. Sagong, Numerical Solution of Singular Two-Point Boundary-Value Problems by Invariant Imbedding, Proceedings of the Third Mexican Workshop on Numerical Analysis, Lecture Notes in Mathematics, Springer-Verlag, Berlin, to appear.

____________________, Invariant Imbedding Applied to Homogeneous Two-Point Boundary-Value Problems with a Singularity of the First Kind, Appl. Math. Comput., to appear.

In Preparation

P. Nelson and S.R. White, Numerical Solution of Singular Inhomogeneous Two-Point Boundary-Value Problems by Invariant Imbedding, in preparation.

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S.R. White, Invariant Imbedding applied to Inhomogeneous Singular Two-Point Boundary-Value Problems, M.S. Report, Department of Mathematics, Texas Tech University, in preparation.

Reports of the Institute for Numerical Transport Theory

INTT-10: Automatic Control of Errors for Invariant Imbedding, by Paul Nelson and Kenneth E. Wiggins (December 1980).

INTT-14: Invariant Imbedding Applied to Homogeneous Two-Point Boundary-Value Problems with a Singularity of the First Kind, by Paul Nelson, Ira T. Elder and Seok Sagong (May 1981).

PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

1) Faculty Investigators: Paul Nelson
Ira T. Elder

2) Graduate Students: Robert Pavur
Seok Sagong
Stevan R. White

INTERACTIONS

Paul Nelson presented an invited paper "Problems and Recent Progress in Invariant Imbedding" at the workshop on Boundary-Value Problems in Ordinary Differential Equations at the University of British Columbia and Simon Fraser University, Vancouver, B.C. (Canada), August 11-14, 1980.

Paul Nelson presented a contributed paper "Numerical Solution of Singular Two-Point Boundary-Value Problems by Invariant Imbedding" at the Third Mexican Workshop on Numerical Analysis, Cocoyoc, Morelos (Mexico), January 12-16, 1981.

Ira T. Elder presented a contributed paper "Invariant Imbedding Applied to Homogeneous Two-Point Boundary-Value Problems with a Singularity of the First Kind" at the 1981 National Meeting of the Society for Industrial and Applied Mathematics, Renesselaer Polytechnic Institute, Troy, New York, June 8-10, 1981.

Paul Nelson discussed applications of invariant imbedding to the problem of computing enhancement of radiation does at material interfaces with Dr. John C. Garth, of the Rome Air Development Center (Hanscom Air Force Base, MA) at the 18th Annual Conference on Nuclear and Space Radiation Effects, University of Washington, Seattle Washington, July 21-24, 1981. These discussions are continuing, and may ultimately lead to collaborative research.

Paul Nelson visited India during the period September 26- October 23, 1981, under the auspices of the U.S.-India Exchange of Scientists Program. During this visit he gave the following lectures which were substantially based on information generated under the subject research effort:

"Recent Progress in the Computational Aspects of Invariant Imbedding" (Indian Institute of Technology, Delhi, September 29; Indian Institute of Technology, Kanpur, September 30; Institute of Mathematical Sciences, Madras, October 19).

"Invariant Imbedding for Singular Two-Point Boundary-Value Problems" (Indian Institute of Technology, Kanpur, October 1; Institute of Mathematical Sciences, Madras, October 20).

"Physical Aspects of Invariant Imbedding" (Kalpakkam Chapter of the Indian Physical Association, October 16).

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